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2007 – present:

- Postdoctoral Research Associate.
- CAAM, Rice University.
- Advisors: William Symes and Tim Warburton.

2001 – 2006:

- Ph.D., Applied Mathematics.
- University of Maryland Baltimore County (UMBC).
- Advisor: Dr. Susan Minkoff.
- Thesis: Operator Upscaling for the Wave Equation.

1995 – 2000:

- M.S., Applied Mathematics
- Kharkiv National University, Ukraine

Numerical Approximation of 1) Infinite Domains, 2) Seismic Sources: What Can We Do?

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Goals and Tools

- **Goal:** Study Finite Differences (FD) and Discontinuous Galerkin (DG) for the wave equation in the seismic context:
  - impact of absorbing boundary conditions,
  - singular sources,
  - discontinuous coefficients (problems with interfaces).

- **Tools for the acoustic wave equation:**
  - DG (2D, C++) (Dr. Warburton).
  - FD (nD, C, OpenMP, MPI) (I. Terentyev).

Outline

- **Part I:** Perfectly Matched Layer (PML).
  - overview,
  - PML for 1D acoustic wave equation,
  - Nearly PML for acoustic wave equation.

- **Part II:** Point Source for Discontinuous Galerkin Method.
  (joint work with Dr. Warburton)
  - linear approximation,
  - trigonometric approximation,
  - adjoint interpolation.

- **Part III:** Dipole Source for Finite Difference Methods.
  - straightforward approximation,
  - smoothed right-hand side,
  - regularization

Model problem: The Acoustic Wave Equation

$$
\begin{aligned}
\frac{1}{\kappa(\mathbf{x})}\frac{\partial p(\mathbf{x},t)}{\partial t} &= -\nabla \cdot \mathbf{v}(\mathbf{x},t), \\
\rho(\mathbf{x})\frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} &= -\nabla p(\mathbf{x},t) + f(t,\mathbf{x}),
\end{aligned}
$$

- p is pressure,
- $\mathbf{v}$ is velocity,
- f is a source,
- κ is bulk modulus,
- ρ is density,
- $t \geq 0$, $\mathbf{x} \in \mathbb{R}^n$.

Initial Conditions

$$
p(0,\mathbf{x}) = p_0(\mathbf{x}), \qquad \mathbf{v}(0,\mathbf{x}) = \mathbf{v}_0(\mathbf{x}).
$$

Infinite Domain?

Absorbing Boundary Conditions

- Goal: Truncate domain without errors.
- Idea: Use artificial boundary with special boundary conditions:
  - **absorbing**,
  - **reflectionless**,
  - accurate (reflection should be less than 1%),
  - stable,
  - cheap,
  - easy to implement.
- Popular approach: Perfectly Matched Layer (PML).

Perfectly Matched Layer (Berenger, 1993)

- **Idea:** Surround the domain by an absorbing medium.
- **Problem:** Reflection coefficient depends on both the angle of incidence and frequency.

Berenger's absorbing layer

no reflections for any frequency and any angle of incidence

$+$

exponential decay with distance into the layer

- **i.e.**: layer is perfectly matched and can itself be truncated.

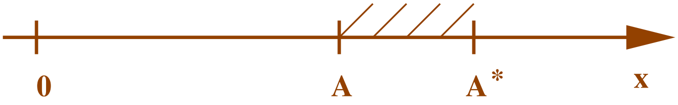
Construction of the PML

- Add damping terms to physical equations.
- Damping terms should vanish in the physical domain.
- Use damping terms to kill waves in the absorbing layer.

PML for 1D Acoustic Problem

- Convert the problem to the frequency domain:

$$
\begin{aligned}
-i\omega\hat{p}(x) + \kappa\frac{\partial\hat{v}(x)}{\partial x} &= 0, \quad 0 < x < A, \\
-i\omega\hat{v}(x) + \frac{1}{\rho}\frac{\partial\hat{p}(x)}{\partial x} &= 0, \quad 0 < x < A.
\end{aligned}
$$



- Choose $\sigma(x) = 0$ for $0 < x < A$ and add dumping terms:

$$
\begin{aligned}
(-i\omega + \sigma(x))\,\hat{p}(x) + \kappa\frac{\partial\hat{v}(x)}{\partial x} &= 0, \quad 0 < x < A^\star, \\
(-i\omega + \sigma(x))\,\hat{v}(x) + \frac{1}{\rho}\frac{\partial\hat{p}(x)}{\partial x} &= 0, \quad 0 < x < A^\star.
\end{aligned}
$$

PML for 1D Acoustic Problem (cont.)

- Eliminate $\hat{v}$, set $\gamma = 1 + i\sigma(x)/\omega$:

$$\frac{\omega^2}{c^2}\hat{p}(x) + \frac{1}{\gamma(x)}\frac{d}{dx}\left(\frac{1}{\gamma(x)}\frac{d}{dx}\hat{p}(x)\right) = 0, \quad 0 < x < A^\star.$$

- Solution to the interface ($x = A$) problem:

$$\hat{p}(x) = \begin{cases} Ie^{ik(x-A)} & + \quad Re^{-ik(x-A)}, \quad 0 < x < A, \\ Te^{ik^\star(x-A)} & + \quad Ce^{-ik^\star(x-A)}, \quad A < x < A^\star \end{cases}$$

with $k = \dfrac{\omega}{c}$ and $k^\star = k\gamma = k + ik\dfrac{\sigma(x)}{\omega}$.

PML for 1D Acoustic Problem (cont.)

$$\hat{p} = \begin{cases} Ie^{ik(x-A)} & + \quad Re^{-ik(x-A)}, & 0 < x < A, \\ Te^{ik(x-A)}e^{-\frac{k}{\omega}\sigma(x)(x-A)} & + \quad Ce^{-ik(x-A)}e^{\frac{k}{\omega}\sigma(x)(x-A)}, & A < x < A^{\star}. \end{cases}$$

- Exponential decay in the pml layer.

PML for 1D Acoustic Problem (cont.)

$$\hat{p} = \begin{cases} Ie^{ik(x-A)} & + \quad Re^{-ik(x-A)}, & 0 < x < A, \\ Te^{ik(x-A)}e^{-\frac{k}{\omega}\sigma(x)(x-A)} & + \quad Ce^{-ik(x-A)}e^{\frac{k}{\omega}\sigma(x)(x-A)}, & A < x < A^{\star}. \end{cases}$$

- Exponential decay in the pml layer.
- All frequencies decay at the same rate ($k = \omega/c \Rightarrow k/\omega = c$).

PML for 1D Acoustic Problem (cont.)

$$\hat{p} = \begin{cases} Ie^{ik(x-A)} & + \quad Re^{-ik(x-A)}, & 0 < x < A, \\ Te^{ik(x-A)}e^{-\frac{k}{\omega}\sigma(x)(x-A)} & + \quad Ce^{-ik(x-A)}e^{\frac{k}{\omega}\sigma(x)(x-A)}, & A < x < A^{\star}. \end{cases}$$

- Exponential decay in the pml layer.
- All frequencies decay at the same rate ($k = \omega/c \Rightarrow k/\omega = c$).
- Boundary condition at $x = A^{\star}$ implies that $C = 0$.

PML for 1D Acoustic Problem (cont.)

$$\hat{p} = \begin{cases} I e^{ik(x-A)} & + \quad R e^{-ik(x-A)}, & 0 < x < A, \\ T e^{ik(x-A)} e^{-\frac{k}{\omega}\sigma(x)(x-A)} & + \quad C e^{-ik(x-A)} e^{\frac{k}{\omega}\sigma(x)(x-A)}, & A < x < A^{\star}. \end{cases}$$

- Exponential decay in the pml layer.
- All frequencies decay at the same rate ($k = \omega/c \Rightarrow k/\omega = c$).
- Boundary condition at $x = A^{\star}$ implies that $C = 0$.
- Continuity of $\hat{p}$ and $\hat{v}$ at $x = A$ implies that

$$\begin{cases} I + R = T, \\ I - R = T, \end{cases} \Rightarrow \begin{cases} R = 0, \\ I = T. \end{cases}$$

(since $-\frac{\kappa}{\omega}\sigma'(x)(x-A) - \frac{\kappa}{\omega}\sigma(x) = 0$ for $x = A$)

PML for 1D Acoustic Problem (cont.)

$$\hat{p} = \begin{cases} I e^{ik(x-A)} & + \quad R e^{-ik(x-A)}, & 0 < x < A, \\ I e^{ik(x-A)} e^{-\frac{k}{\omega}\sigma(x)(x-A)} & + \quad C e^{-ik(x-A)} e^{\frac{k}{\omega}\sigma(x)(x-A)}, & A < x < A^{\star}. \end{cases}$$

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  (since $-\frac{\kappa}{\omega}\sigma'(x)(x-A) - \frac{\kappa}{\omega}\sigma(x) = 0$ for $x = A$)
- After discretization the reflection coefficient is not zero, but is small ,provided that the discrete scheme is accurate.

Nearly PML (NPML) for 2D acoustic equation

$$\frac{1}{\kappa}\frac{\partial p}{\partial t} + \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial x} = 0,$$
$$\rho\frac{\partial v_x}{\partial t} + \frac{\partial p}{\partial x} = 0,$$
$$\rho\frac{\partial v_y}{\partial t} + \frac{\partial p}{\partial y} = 0.$$

PML vs. NPML

- NPML is less expensive and easier to implement (Cummer 2003)
- mathematically equivalent

NPML Formulation

$$\frac{1}{\kappa}\frac{\partial p}{\partial t} + \frac{\partial \bar{v}_x}{\partial x} + \frac{\partial \bar{v}_y}{\partial x} = 0,$$

$$\frac{\partial \bar{p}_x}{\partial t} + \sigma(x)\bar{p}_x = \frac{\partial p}{\partial t},$$
$$\frac{\partial \bar{p}_y}{\partial t} + \sigma(y)\bar{p}_y = \frac{\partial p}{\partial t},$$

$$\rho\frac{\partial v_x}{\partial t} + \frac{\partial \bar{p}_x}{\partial x} = 0,$$
$$\rho\frac{\partial v_y}{\partial t} + \frac{\partial \bar{p}_y}{\partial y} = 0,$$

$$\frac{\partial \bar{v}_x}{\partial t} + \sigma(x)\bar{v}_x = \frac{\partial v_x}{\partial t},$$
$$\frac{\partial \bar{v}_y}{\partial t} + \sigma(y)\bar{v}_y = \frac{\partial v_y}{\partial t}.$$

Nearly PML (NPML) for 2D acoustic equation

- 2D: 9 domains, 7 variables
- 3D: 27 domains, 10 variables
- Igor's modification:
  - 2D: 4 variables
  - 3D: 6 variables

all 7	P V_x V_y $\overline{P}_y$ $\overline{V}_y$	all 7
P V_x V_y $\overline{P}_x$ $\overline{V}_x$	P V_x V_y	P V_x V_y $\overline{P}_x$ $\overline{V}_x$
all 7	P V_x V_y $\overline{P}_y$ $\overline{V}_y$	all 7

NPML Formulation

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Nearly PML (NPML) for 2D acoustic equation

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all 7	P V_x V_y $\overline{P}_y$ $\overline{V}_y$	all 7

NPML Formulation

$$\frac{1}{\kappa}\frac{\partial p}{\partial t} + \frac{\partial \bar{v}_x}{\partial x} + \frac{\partial \bar{v}_y}{\partial x} = 0,$$

$$\frac{\partial \bar{p}_x}{\partial t} + \sigma(x)\bar{p}_x = \frac{\partial p}{\partial t},$$
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$$\rho\frac{\partial v_x}{\partial t} + \frac{\partial \bar{p}_x}{\partial x} = 0,$$
$$\rho\frac{\partial v_y}{\partial t} + \frac{\partial \bar{p}_y}{\partial y} = 0,$$

$$\frac{\partial \bar{v}_x}{\partial t} + \sigma(x)\bar{v}_x = \frac{\partial v_x}{\partial t},$$
$$\frac{\partial \bar{v}_y}{\partial t} + \sigma(y)\bar{v}_y = \frac{\partial v_y}{\partial t}.$$

Numerical Example

play

Error (float)

- Homogeneous medium $\rho = 1$, $\kappa = 1$.
- Size of the domain $\Omega = [-2, 2] \times [-2, 2]$.
- Absorbing layer is two-wavelength wide.

$nx \times nz$	$h_x = h_z$	$\|\|p_h - p\|\|_{\mathrm{inf}}$
100×100	0.04	4.118e-04
200×200	0.02	4.048e-04
400×400	0.01	4.043e-04
800×800	0.005	4.043e-04
1600×1600	0.0125	4.043e-04

- PML gives accurate results at acceptable computational cost.

Parts II and III: Numerical Approximation of Singular Sources

First step: Code validation by means of convergence tests:

- smooth source, const coefficients: optimal order for DG & FD,
- singular source, const coefficients,
- singular source, discontinuous coefficients.

DG: Point Source

- Acoustic problem with point source scaled by Ricker's wavelet:

$$\begin{aligned} \frac{\partial p(\mathbf{x},t)}{\partial t} &= -\nabla \cdot \mathbf{v}(\mathbf{x},t) + f(t)\delta(\mathbf{x}), \\ \frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} &= -c(\mathbf{x})^2 \nabla p(\mathbf{x},t), \end{aligned}$$

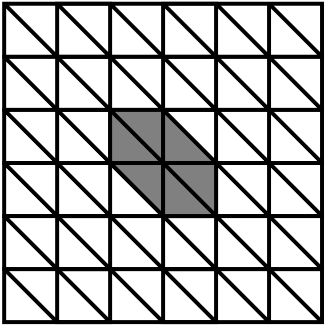
- Analytical solution is given by Poisson's formula:

$$\begin{aligned} p(\mathbf{x},t) &= \frac{1}{2\pi c^3} \int_0^t f'(\tau) \int_{U(\mathbf{x};c(t-\tau))} \frac{\delta(\boldsymbol{\xi}) d\boldsymbol{\xi}}{\sqrt{c^2(t-\tau)^2 - |\mathbf{x}-\boldsymbol{\xi}|^2}} d\tau \\ &= \frac{1}{\pi c^4} \int_0^{\sqrt{t-|\mathbf{x}|/c}} \frac{f'(t-|\mathbf{x}|/c-\tau^2)}{\sqrt{\tau^2 + 2|\mathbf{x}|/c}} d\tau. \end{aligned}$$

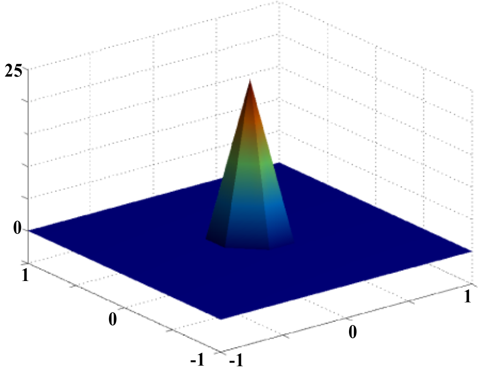
- Gaussian 8-node adaptive quadrature (I. Terentyev).

Linear Approximation: $\int \delta(x)dx = 1$

Support

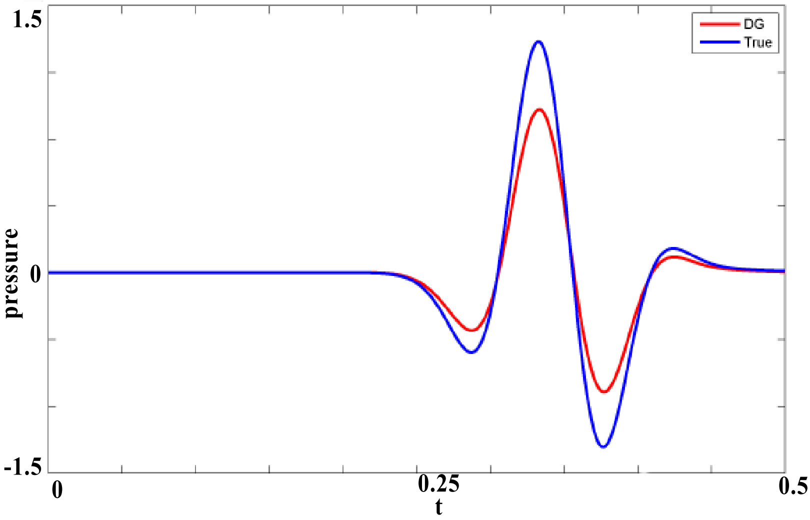


Linear approximation

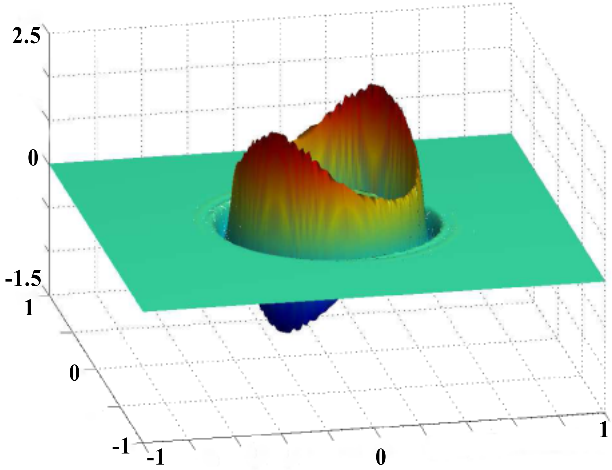


Linear Approximation of the Delta Function (cont.)

Traces of the numerical solution (red) and reference solution (blue)

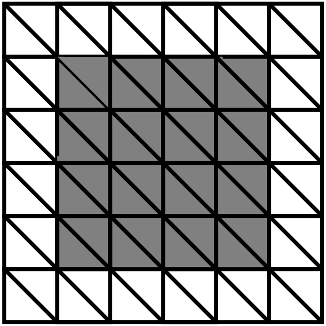


Numerical Solution

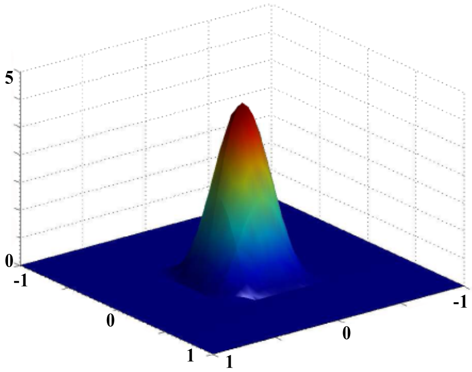


Trigonometric Approximation: $\int \delta(x)dx = 1$

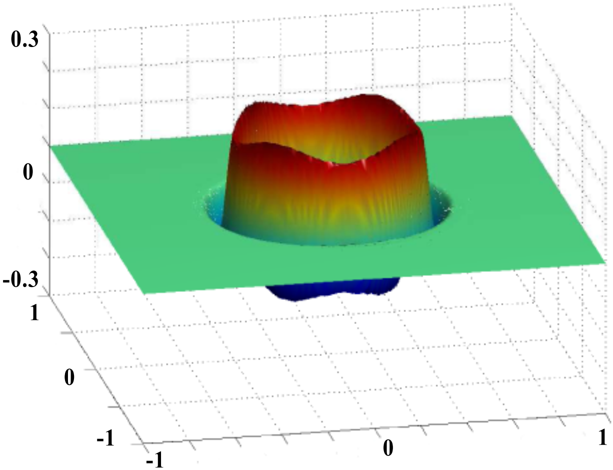
Support



Trigonometric approximation

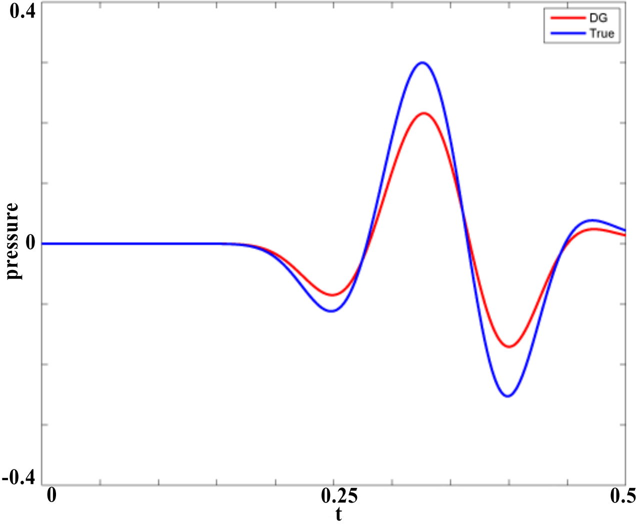


Numerical Solution

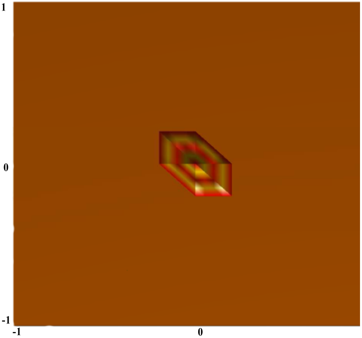


Trigonometric Approximation of the Delta Function (cont.)

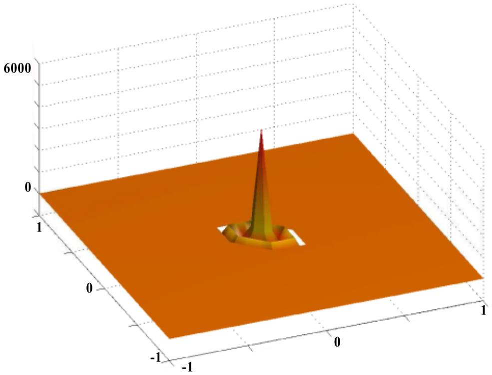
Traces of the numerical solution (red) and reference solution (blue)



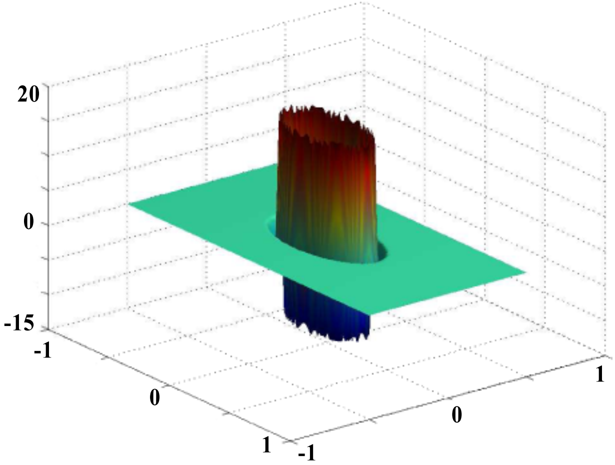
Support



FE approximation

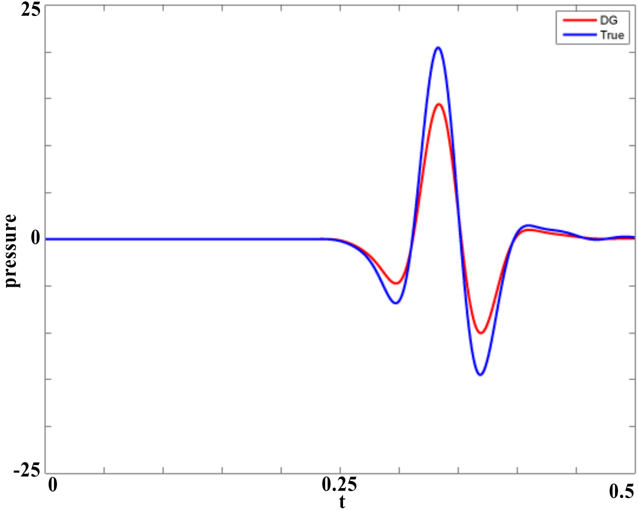


Numerical Solution



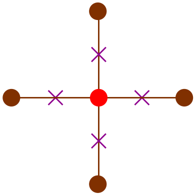
FE Approximation of the Delta Function (cont.)

Traces of the numerical solution (red) and reference solution (blue)



FDM: Dipole Source

- Acoustic problem with diplole source scaled by Gaussian:



$$
\begin{aligned}
\frac{1}{\kappa(\mathbf{x})}\frac{\partial p(\mathbf{x},t)}{\partial t} &= -\nabla\cdot\mathbf{v}(\mathbf{x},t),\\
\rho(\mathbf{x})\frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} &= -\nabla p(\mathbf{x},t)+\mathbf{f}(t)\nabla\delta(\mathbf{x}),
\end{aligned}
$$

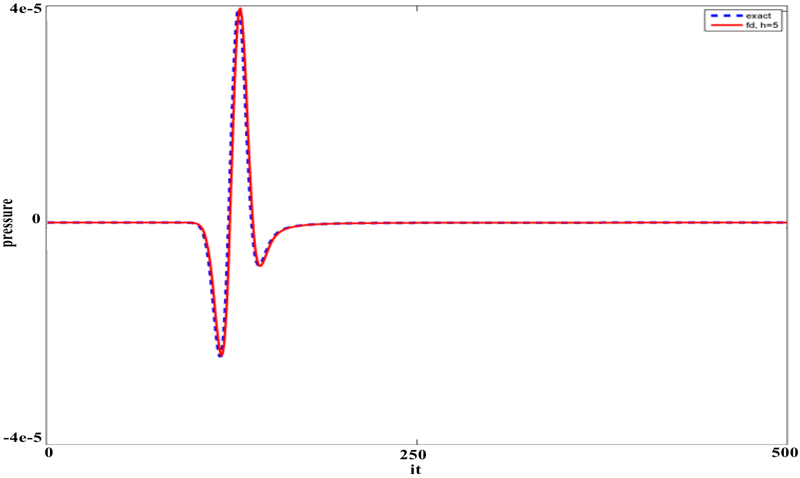
- Analytical solution is given by Poisson's formula:

$$
p(\mathbf{x},t) = -\frac{1}{\pi c^2}\int_0^{\sqrt{t-|\mathbf{x}|/c}} \frac{f''(t-|\mathbf{x}|/c-\tau^2)}{\sqrt{\tau^2+2|\mathbf{x}|/c}}\,d\tau.
$$

- 2-4 staggered finite differences scheme.

Numerical results for the Dipole Problem

Traces of the numerical solution (blue) and reference solution (red)



Error (floats) and Rate of Convergence

- Naive approximation of the dipole is reasonably accurate.
- No point-wise convergence.

$nx \times nz$	$h_x = h_z$	$\|\|p_h - p\|\|_{\text{inf}}$	$\frac{\|\|p_h - p\|\|_{\text{inf}}}{\|\|p\|\|_{\text{inf}}}$
500×500	10	4.502e-07	1.131e-02
1000×1000	5	3.057e-07	7.684e-03
2000×2000	2.5	3.025e-07	7.602e-03
4000×4000	1.25	3.227e-07	8.112e-03
8000×8000	0.625	4.775e-07	1.200e-02

- The solution is smooth away from the source location.
- **Idea:** construct a "smooth" problem that away from the source gives us a solution equivalent to the solution of the dipole problem.

Smoothed Source Functions

Let

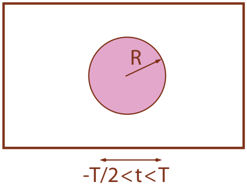
- $(p, \mathbf{v})$ solve the dipole problem in Ω for $-T/2 < t < T_0$,
- $(p_s, \mathbf{v}_s)$ solve the problem with the smoothed source functions $F_p(\mathbf{x}, t)$ and $\mathbf{F}_v(\mathbf{x}, t)$ in Ω for $-T/2 < t < T_0$.

Then

- $(p, \mathbf{v})$ and $(p_s, \mathbf{v}_s)$ are equivalent for $||\mathbf{x} - \mathbf{x}_s|| > R$ and $t > T$,

provided that

- source wavelet $f(t)$ vanishes for $|t| > T/2$,
- $\kappa(\mathbf{x}) = \kappa_s$, $\rho(\mathbf{x}) = \rho_s$ in a region of radius R about source $\mathbf{x}_s$.

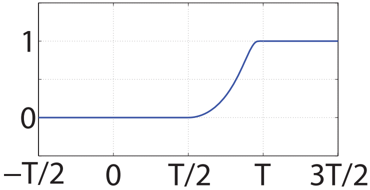


Construction of Smoothed Source Functions (2D)

$$F_p(\mathbf{x},t) = \frac{1}{\kappa_s} p_0(\mathbf{x},t)\frac{\partial \phi(t)}{\partial t} \quad \text{and} \quad \mathbf{F}_v(\mathbf{x},t) = \rho_s \mathbf{v}_0(\mathbf{x},t)\frac{\partial \phi(t)}{\partial t},$$

where

- $p_0(\mathbf{x},t) = -\frac{1}{\pi c_s^2}\int_0^{\sqrt{t-|\mathbf{x}|/c_s}} \frac{f''(t-|\mathbf{x}|/c_s-\tau^2)}{\sqrt{\tau^2+2|\mathbf{x}|/c_s}}\,d\tau,$
- $\mathbf{v}_0(\mathbf{x},t) = -\frac{1}{\rho_s}\int_0^t \nabla p_0(\mathbf{x},\tau)\,d\tau,$
- $\phi(t) =$



Error (floats) and Rate of Convergence (2D)

- Appears to converge with optimal rate.

$nx \times nz$	$h_x = h_z$	$\frac{\|\|p_h - p\|\|_{\text{inf}}}{\|\|p\|\|_{\text{inf}}}$	Rate
250×250	20	4.689e-06	–
500×500	10	6.856e-07	6.83
1000×1000	5	2.041e-07	3.35
2000×2000	2.5	5.329e-08	3.83
4000×4000	1.25	–	–

- Too slow in 2D (about 5 days for 2000×2000 problem).
- Acceptably fast in 3D (no numerical integration).
- Limitation: homogeneity assumption around the source.

Regularization of Singular Sources

- **Elliptic problems:** Peskin (1977), Beyer & LeVeque (1992), Tornberg & Engquist (2002)
- **Idea:** replace $\delta(x)$ with discrete approximation $d_h(x)$ that
  - has bounded support,
  - satisfies vanishing moment conditions:

$$\sum_j d_h(x_j) = 1 \text{ and } \sum_j x_j^m d_h(x_j) = \delta_{m0} \text{ for } m = 1, \ldots, p.$$

- **Result:** Error is determined by the order of the difference scheme and number of moment conditions satisfied by the discrete delta function.
- **Hyperbolic systems in 1D with discontinuous initial data:** Lax ('06) optimal weak convergence for initial data smoothed by averaging kernel that satisfies moment conditions.

2, 2k order staggered scheme for the dipole problem

$$
\begin{aligned}
M(V_{n+1/2} - V_{n-1/2}) &= -\lambda D P_n + \Delta t F_n, \\
K^{-1}(P_{n+1} - P_n) &= \lambda D^T V_{n+1/2},
\end{aligned}
$$

where

- $V_{n+1/2}$ and P_{n+1} are velocity and pressure grid vectors,
- M and K are diagonal density and bulk modulus matrices,
- D is undivided difference operator,
- $F_n = f(n\Delta t) D d_h(i + 1/2)$ is a source.

- Discrete energy inner product:

$$
\left\langle \begin{pmatrix} V^1 \\ P^1 \end{pmatrix}, \begin{pmatrix} V^2 \\ P^2 \end{pmatrix} \right\rangle_E = \langle V^1, M V^2 \rangle + \langle P^1, K^{-1} P^2 \rangle
$$

$$
-\frac{\lambda}{2} \left(\langle V^1, D P^2 \rangle + \langle V^2, D P^1 \rangle \right).
$$

Regularization Result

Assume

- $(\mathbf{v}, p)$ solve the dipole problem,
- $(\bar{\mathbf{v}}, \bar{p})$ solve the time-reversed problem with smooth source,
- $(V_{n+1/2}, P_{n+1})$ solve the discrete dipole problem,
- $(\bar{V}_{n+1/2}, \bar{P}_{n+1})$ solve the discrete time-reversed problem,
- discrete delta function d_h satisfies appropriate number of moment conditions.

Then for $T = (N+1)\Delta t$

$$\left(\begin{pmatrix} \mathbf{v}(T) \\ p(T) \end{pmatrix}, \begin{pmatrix} \bar{\mathbf{v}}(T) \\ \bar{p}(T) \end{pmatrix} \right)_{\mathcal{E}} = \left\langle \begin{pmatrix} V_{N+1/2} \\ P_{N+1} \end{pmatrix}, \begin{pmatrix} \bar{V}_{N+1/2} \\ \bar{P}_{N+1} \end{pmatrix} \right\rangle_E + O(\Delta t^2 + h^2),$$

where $\left(\begin{pmatrix} \mathbf{v}(T) \\ p(T) \end{pmatrix}, \begin{pmatrix} \bar{\mathbf{v}}(T) \\ \bar{p}(T) \end{pmatrix} \right)_{\mathcal{E}} = (\mathbf{v}, \rho\bar{v})_{L^2} + (p, \kappa^{-1}\bar{p})_{L^2}.$

Summary

- Nearly Perfectly Matched Layer (NPML) for staggered finite-difference methods combines reasonable accuracy and acceptable computational cost.

- Straightforward approximations of point and dipole sources converge only weakly (if at all).

- Can we recover strong convergence?
  - regularization (analytical smoothing),
  - adaptive mesh refinement?
  - other approaches? Stay tuned...